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# Benchmarking the PAWN Distribution-based Method Against the Variance-based Method in Global Sensitivity Analysis: Empirical Results

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## Abstract

The search for new and more efficient global sensitivity analysis methods has led to the development of the PAWN distribution-based method. This method has been proven to overcome one of the main limitation of variance-based methods – the moment independent property. In this regard, the distribution-based method has outperformed the variance-based method for some highly-skewed or multi-modal distributions. However, despite its increasing popularity, there is a lack of understanding about the performance and properties of the distribution-based method. The benchmark presented in this paper is an attempt to remedy this. We compare the distribution-based method against the variance-based method for a set of well-known test functions. We show that, whereas the distribution-based method can be used as a complementary approach to variance-based methods, which is especially useful when dealing with highly-skewed or multi-modal distributions, it fails to rank different inputs that have different orders of magnitude in their contribution of the response.

**Keywords:** Global sensitivity analysis, PAWN distribution-based method, variance-based sensitivity analysis

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# 1 Introduction

Global Sensitivity Analysis (GSA) methods are used to study how different sources of uncertainty in model output can be apportioned to the different sources of uncertainty in model input by exploring the combined space formed by all parameters in the domain [1] [2]. Before starting a GSA, it is imperative to define which research question needs to be answered and which risk metrics are to be used to quantify uncertainty. Different research questions and risk metrics will lead to different answers, and therefore this is something that has to be established from the very beginning.

In the context of this paper, the research question GSA attempts to answer is to determine the most relevant input variables to an output behaviour, as well as to identify those variables whose contribution can be neglected. By ranking the model inputs in order of importance, useful insights into the model can be gained, especially when the system is not well known or the model is in the early stages of development. The process of ranking these inputs is also referred to as **Factor Prioritization**[2]. Prioritization leads naturally to the idea of important inputs but also to negligible inputs or factors whose variability has a negligible effect on the output. Very often the inputs into a model follow very asymmetric distributions of importance, with few inputs accounting for most of the output uncertainty and most inputs playing little or no role [3]. By identifying those parameters that have no significant contribution to the model output, the complexity of the model can be reduced. This is also known as **Factor Fixing**[2].

It is similarly important to define the risk metric. A number of methods have been developed. One of the most well-established and extensively used GSA method is the Sobol or variance-based method, developed in 1990 by Ilya Meyerovich Sobol [4]. The Sobol method decomposes the variance of the model output in terms of the input variances. The method is model independent and therefore, it can be applied to any model regardless of the response function of the input-outputs. In addition, it is easy to interpret and to implement, making it the cornerstone of GSA. However, one of the key limitations of the method concerns the fact that the method needs a moment of the output distribution to fully characterize the output uncertainty.

Moment independent techniques arose from the works of Borgonovo [5] and Liu [6], where highly-skewed distributions were analysed to examine how its variance is decomposed. When using conventional variance-based GSA techniques both works concluded that identifying variance with uncertainty might lead to misleading conclusions. The first set of results showed that the unconditional variance was lower than the conditional variance at a given conditioning value, implying that the variance of the output increases when removing the uncertainty from one of the inputs; an example of that can be found in [2] for non-additive models. The second example failed to rank the importance of the different input uncertainties. Therefore, decision makers might be given a false sense of security, whereby attempting to fix/reduce some of the input uncertainty may result in higher variability of the output. These findings prompted the research community to investigate methods that remove the dependence on a single moment. As such, moment independent techniques are not affected by the presence of correlations and can provide a solution for those distributions that are not well represented by its variance, avoiding costly pitfalls.

As a consequence, several GSA methods were developed (citing here just a few) such as the entropy-based and the  $\delta$ -sensitivity to overcome the moment dependent property [5, 6]. However, the practical implementation of those methods has been quite limited [7]. This is thought to be related with the computational cost of calculating many Probability Distribution Functions (PDFs). Later on, the PAWN method was published in 2015, coined under the name of “A simple and efficient method for GSA based on CDFs” [7]. The innovative idea was to use the Cumulative Distribution Function (CDF) instead of the PDF in order to apportion the uncertainty of the output into the different inputs. The underlying reason for choosing CDFs over PDFs is based on the fact that CDFs are much easier to

approximate than PDFs [7]. PDFs are usually unknown and must be estimated empirically. An easier way to calculate an empirical PDF would be to use a histogram of the data sample, whose resulting shape will be conditioned on both the position of the first bin and the size of the bin. However, obtaining values that correctly represent the empirical PDF may be difficult. A different way to estimate the PDFs would be to use the Kernel Density Estimation (KDE) methods, which would only require the estimation of a single parameter – the bandwidth. Another approach that has been used in the past is to first estimate the CDFs, and then use derivation techniques to work out the empirical PDFs [6]. Given that the calculation of PDFs has to be repeated many times, it must be as computationally inexpensive as possible. As a result, it seems logical to compute CDFs instead of PDFs at no extra cost and without the need for tuning parameters. Not only does the PAWN method claimed to address the complexity of previous moment independent methods; its authors also provided several examples where the method outperforms the variance-based method for those PDF model output distributions that were highly-skewed or multi-modal, suggesting that, in these cases, variance was not a good proxy for uncertainty.

Findings that more theoretical understanding is needed in order to employ CDF-based sensitivity measures are available in the existing literature as shown in [8, 9, 10]. Nevertheless, given its advantages, moment independent techniques are continuously being applied to tackle complex problems. In 2016 the PAWN method was used in a techno-economic optimal wind-energy converter, where its model exhibited an output PDF which was not symmetric but right-skewed [11]. As a result, negative values were obtained for those cases where the conditional variance exceeded the unconditional variance; result of which was driven by a numerical approximation due to the limited sample size. In 2017, the Sobol and PAWN GSA techniques were compared for a hydrological model called Soil and Water Assessment Tool [12]. The comparison was undertaken in terms of the convergence rate, parameter ranking and screening results. It was shown that there were no differences between the two methods as for the convergence rate and screening results. However, PAWN and Sobol came up with a different ranking of the model inputs importance. The paper emphasised that this was due to the underlying assumption that Sobol considers variance as a good proxy for uncertainty, whereas in reality this may not be the case; at the same time the paper suggested that the variance-based and PAWN methods may be regarded as complementary approaches to study the sensitivity of model output.

Although the PAWN method has been widely adopted, a major limitation of PAWN was perceived by the authors regarding the need for a tailored sampling strategy to approximate the sensitivity indices. PAWN required to tune the triplet  $Nu$ ,  $Nc$  and  $n$  to compute its PAWN indices. However, no one has yet analysed how to choose the values for the triplet. In addition, given the tailored sampling strategy, it is difficult to apply several GSA methods to the same problem, as PAWN requires dedicated model evaluations. In 2018, the authors addressed these two issues by developing a generic approach of the PAWN method, called the distribution-based global sensitivity analysis. This generic approach provides a solution for these two limitations as shown in [13]. On a separate note, Gamboa et al. investigated in 2018 the generalisation of the so-called Sobol indices to higher moments, where its index appears to be more general than Sobol as it takes into consideration the whole distribution and not the second moment [14].

Given the number of people that use the PAWN distribution-based method in the field of environmental modelling [22], the authors would like to limit the scope of this paper to benchmark the PAWN distribution-based against the variance based. Even though the one from Gamboa is well suited for this comparison, this will be considered in future work. Further research is necessary to compare the PAWN distribution-based method against the well-established Sobol method, before the former can be widely adopted by the community. Therefore, a wider set of reference test functions has to be used to benchmark these two methods for those cases where the analytical variances of the test functions are known. In other words, the community needs to know how the PAWN distribution-based method compares to Sobol for those cases where Sobol has worked well and also which are the advantages

of the PAWN distribution-based over Sobol. The aim of the current paper is to remedy this lack of understanding by providing this benchmark. We then show its properties, and suggest where the method is appropriate.

The rest of this paper is organised as follows: Section 2 and 3 introduces the fundamentals of variance-based and PAWN distribution-based GSA, respectively. Following this, a set of well-known test functions is introduced in Section 4 and used to benchmark the two methods. Results and discussions are shown in Section 5. Conclusions are drawn in Section 6.

## 2 Sobol method

### 2.1 Introduction

The Sobol method, or variance-based sensitivity analysis, is a form of global sensitivity analysis that focus on decomposing the variance of the model outputs in terms of the variance of the model inputs. The following formulation is reproduced from [4]. Let us assume that a mathematical model can be represented by Equation 1, which is made of summands of increased dimensionality. This is also called a High Dimensional Model Representation (HDMR), where the total number of summands in Equation 1 is  $2^N$ . Let us also consider that the model input  $\mathbf{X}$  belongs to the  $n$ -dimensional unit hypercube domain  $I^N$ , which is expressed as:  $X_i \in [0, 1] \forall i \in 1, \dots, N$ .  $f(\mathbf{X})$  is the model under study and the number of elements of increasing dimensionality grows as a function of  $\binom{N}{i} \forall i \in 1, \dots, N$ .

$$Y = f(\mathbf{X}) = f_0 + \sum_i f_i(X_i) + \sum_{i < j} f_{i < j}(X_i, X_j) + \dots + f_{12\dots n}(X_1, X_2, \dots, X_N) \quad (1)$$

As a result, the total number of summands (apart from  $f_0$ ) is given by Equation 2.

$$\sum_{i=1}^N \binom{N}{i} = 2^N - 1 \quad (2)$$

If the following requirement in Equation 3 can be satisfied, then the representation of the model is called Analysis of Variance (ANOVA) HDMR. This means that the variables are considered to be mutually independent and it has been proven that this decomposition is unique [15].

$$\int_0^1 f_{i_1 \dots i_s} dX_k = 0 \quad \text{for } k = i_1, \dots, i_s \quad (3)$$

From assumption 3 and Equation 1, it follows the following relationships 4 to 7, where  $X_i$  is the  $i$ -th factor,  $X_{\sim i}$  denotes all the factors but the  $i$ -th and  $\mathbf{E}$  is the expectation operator.

$$\mathbf{E}[Y] = \int_{I^N} f(\mathbf{X}) = f_0 \quad (4)$$

$$\mathbf{E}_{\mathbf{X}_{\sim i}}[Y|X_i] = \int_{I^N} f(\mathbf{X}) \prod_{k \neq i} dX_k = f_0 + f_i(X_i) \quad (5)$$

$$\mathbf{E}_{\mathbf{X}_{\sim i,j}}[Y|X_i, X_j] = \int_{I^N} f(\mathbf{X}) \prod_{k \neq i,j} dX_k = f_0 + f_i(X_i) + f_j(X_j) + f_{ij}(X_i, X_j) \quad (6)$$

$$\begin{aligned} \mathbf{E}_{\mathbf{X} \sim i,j,1}[Y|X_i, X_j, X_l] = \int_{I^N} f(\mathbf{X}) \prod_{k \neq i,j,l} dX_k = f_0 + f_i(X_i) + f_j(X_j) + f_l(X_l) + \\ f_{ij}(X_i, X_j) + f_{il}(X_i, X_l) + f_{jl}(X_j, X_l) + f_{ijl}(X_i, X_j, X_l) \end{aligned} \quad (7)$$

Equation 4 shows that, when integrating the HDMR, all the terms cancel out apart from the constant  $f_0$ . The differential  $\times dX_k \forall k \in 1, \dots, N$  concerns the integration of the model respect those  $k$  variables. It becomes apparent that when fixing a variable, the integration does not lead to a 0 contribution as per assumption 3. The procedure is continued until all  $(N - 1)$ -dimensional summands are defined, and then for the last member  $f_{12\dots N}(X_1, X_2, \dots, X_N)$  Equation 1 is used. By regrouping the terms and calculating the multidimensional integrals, the different HDMR functions can be obtained in a recursive way.

## 2.2 Construction of ANOVA in HDMR

If we now assume that the input parameters are independent random variables uniformly distributed over  $[0, 1]$ , as expressed in 8, as well as that  $f(\mathbf{X})$  is square integrable (so are all the terms), then the following Equations hold. The expectation of this function is given in Equation 9, where  $f_X(\mathbf{X})$  is the pdf of  $\mathbf{x}$  and by construction this is equal to 1.

$$\mathbf{X} = \{X_1, \dots, X_N^T\}, X_i \sim \mathcal{U}(0, 1), \forall i \in 1, \dots, N \quad (8)$$

$$\mathbf{E}[f(X)] = \int_{I^N} f(\mathbf{X}) f_X(\mathbf{X}) d\mathbf{X} = \int_{I^N} f(\mathbf{X}) d\mathbf{X} = f_0 \quad (9)$$

The total variance of the function can be defined in Equation 10.

$$\mathbf{V}[Y] = \int f(\mathbf{X})^2 d\mathbf{X} - f_0^2 \quad (10)$$

Taking the different functional components of the HDMR  $\{f_0, f_i, f_{ij}, \dots\}$ , partial variances  $V_i, V_{ij}$  can be calculated as in Equations 11 and 12. In addition, the total variance  $V(Y)$  can be decomposed using Equation 13.

$$V_i = V(f_i(X_i)) = \mathbf{V}_{X_i}(\mathbf{E}_{\mathbf{X} \sim i}[Y|X_i]) \quad (11)$$

$$V_{ij} = V(f_{ij}(X_i, X_j)) = \mathbf{V}_{X_i X_j}(\mathbf{E}_{\mathbf{X} \sim ij}[Y|X_i, X_j]) - \mathbf{V}_{X_i}(\mathbf{E}_{\mathbf{X} \sim i}[Y|X_i]) - \mathbf{V}_{X_j}(\mathbf{E}_{\mathbf{X} \sim j}[Y|X_j]) \quad (12)$$

$$\mathbf{V}[Y] = \sum_i V_i + \sum_{i < j} V_{ij} + \dots + V_{12\dots n} \quad (13)$$

### 2.3 Sensitivity indices

The decomposition of variance used in the previous section allows to define the following sensitivity analysis indices: the first and total order sensitivity coefficients. Whereas the first order  $S_i$  coefficient measures the part of variance which is caused by  $X_i$ , it does not take into account the interaction with the other variables. When considering the order 2 coefficient  $S_{ij}$ , it not only takes into account the part of variance caused by  $X_i$  and  $X_j$ , but also the interaction between  $X_i$  and  $X_j$ . The order 3 sensitivity coefficient  $S_{ijk}$  includes the variance of the output  $Y$ , resulting from the interactions of the three variables  $X_i$ ,  $X_j$  and  $X_k$ , which is not explained by neither considering the single variables nor by the interaction of two variables. This can be generalised until the highest order.

The first sensitivity index is defined in Equation 14. Regardless of the interactions in the model,  $S_i$  is a measure of the main effect. In other words, it gives information on how much output variance could be reduced when fixing the input model  $X_i$ .

$$S_i = \frac{\mathbf{V}_{X_i}(\mathbf{E}_{\mathbf{X}_{\sim i}}[Y|X_i])}{V(Y)} = \frac{V_i}{V(Y)} \quad (14)$$

Where  $X_i$  is the  $i$ -th factor and  $X_{\sim i}$  denotes all the factors but the  $i$ -th. The expectation of  $Y$  is taken over all the possible values of  $X_{\sim i}$  while keeping  $X_i$  fixed. The outer variance is taken over all possible values of  $X_i$ . Although the total effects  $S_{T_i}$  are a direct consequence from Sobol's decomposition, they weren't explicitly mentioned until the work of Homma and Saltelli [16]. It is worth remembering that the number of coefficients to be computed grows exponentially according to  $2^N$ , where  $N$  is the number of uncertain variables. Consequently, computing all Sobol components can be prohibitive if the model has many inputs. For this reason, and as a means to overcome this challenge, the total effect index was introduced, as defined in Equation 15. The total effect index takes into account the total contribution of the output variation due to the factor  $X_i$ , which includes the first-order effect as well as all higher-order interactions.

$$S_{T_i} = 1 - S_{\sim i} \quad (15)$$

Where  $S_{\sim i}$  is the sum of all  $S_{i_1 \dots i_s}$  that do not include the index  $i$ . A different formalism for it is shown in Equation 16 as in the work of Sudret [17].

$$S_{T_i} = \sum_{I_i} \frac{V_{i_1 \dots i_s}}{V(Y)} \quad I_i = \{\{i_1, \dots, i_s\} \supset \{i\}\} \quad (16)$$

In order to be consistent with the first order mathematical definition, the total order index can be defined in Equation 17.

$$S_{T_i} = \frac{\mathbf{E}_{\mathbf{X}_{\sim i}}(\mathbf{V}_{X_i}([Y|X_{\sim i}]))}{V(Y)} = 1 - \frac{\mathbf{V}_{\mathbf{X}_{\sim i}}(\mathbf{E}_{X_i}([Y|X_{\sim i}]))}{V(Y)} \quad (17)$$

As described in [18], a way to visualise the total order index is to consider  $\mathbf{V}_{\mathbf{X}_{\sim i}}(\mathbf{E}_{X_i}([Y|X_{\sim i}]))$  as the first effect order of the  $X_{\sim i}$ . If we were to subtract this value from  $V(Y)$ , this would mean that the remaining variance should be the contribution of all terms in the decomposition that include  $X_i$ .



A summary of the different statistical measures and its interpretations is given in table 1. It is important to notice that the Law of Total Variance can be applied for 1&4 as well as 2&3.

Table 1: Statistical measures and interpretation

ID	Mathematical notation	Interpretation
1	$\mathbf{V}_{X_i}(\mathbf{E}_{\mathbf{X}_{\sim i}}[Y X_i])$	Expected reduction in variance that would be obtained if $x_i$ could be fixed.
2	$\mathbf{E}_{\mathbf{X}_{\sim i}}(\mathbf{V}_{X_i}([Y X_{\sim i}]$	Expected variance that would be left if all factors but $x_i$ could be fixed.
3	$\mathbf{V}_{X_{\sim i}}(\mathbf{E}_{\mathbf{X}_i}[Y X_{\sim i}])$	Expected variance that would be obtained if all factors but $x_i$ could be fixed.
4	$\mathbf{E}_{\mathbf{X}_i}(\mathbf{V}_{X_{\sim i}}([Y X_i])$	Expected reduction in variance that would be left if $x_i$ could be fixed.

## 2.4 Latest results on the Sobol method

Since Sobol first published his work, many different estimators have appeared in the literature attempting to increase the efficiency of the method in computing the sensitivity indices. The latest estimators and designs are found in [18] [19]: the radial sampling versus the winding stairs. These show that a radial design outperforms winding stairs. Therefore, this paper also adopts the same principle as a comparator.

Given two independent sampling matrices  $\mathbf{A}$  and  $\mathbf{B}$ ,  $a_{ji}$  and  $b_{ji}$  are the generic elements of the matrices, where  $j$  is a dummy variables that varies from one to the number of simulations ( $N$ ) and  $i$  is a second dummy variable that varies between one and the number of input variables ( $k$ ). The generic elements of the matrix are obtained using Sobol's quasi-random numbers, or the so-called shifted  $LP_t$  sequences. The use of these low discrepancy series speeds up the performance of conventional Monte Carlo sampling. There are open-source libraries that generate this sequences based on [20]. We can now define  $\mathbf{A}_{\mathbf{B}}^{(i)}$  as the matrix  $\mathbf{A}$ , where the only difference is that column  $i$  belongs to  $\mathbf{B}$ . By using the notation at matrix or component level, the total sensitivity indices  $S_{T_i}$  are estimated by Jansen [21] and displayed in 18 and 19 respectively.

$$\mathbf{E}_{\mathbf{X}_{\sim i}}(\mathbf{V}_{X_i}([Y|X_{\sim i}])) = \frac{1}{2N} \sum_{j=1}^N [f(\mathbf{A})_j - f(\mathbf{A}_{\mathbf{B}}^{(i)})_j]^2 \quad (18)$$

$$\mathbf{E}_{\mathbf{X}_{\sim i}}(\mathbf{V}_{X_i}([Y|X_{\sim i}])) = \frac{1}{2N} \sum_{j=1}^N [y(a_1^{(j)}, a_2^{(j)}, \dots, a_k^{(j)}) - y(a_1^{(j)}, a_2^{(j)}, \dots, b_i^{(j)}, \dots, a_k^{(j)})]^2 \quad (19)$$

Further information and details on the implementation of Sobol can be found in [18] [19].

### 3 Distribution-based method

#### 3.1 Introduction

We now describe the distribution-based method. The unconditional cumulative distribution function (UCDF) of the output  $y$  is represented by  $F_y(y)$ , whereas the conditional cumulative distribution function (CCDF) of the output when  $x_i$  has been fixed is represented by  $F_{y|x_i}(y)$ . The logic behind this GSA technique consists of assessing the distance between  $F_y(y)$  and  $F_{y|x_i}(y)$ ; this distance accounts for the variability of the output that has been reduced due to fixing variable  $x_i$ , providing an importance measure of  $x_i$  on the output.

Let us imagine that  $F_y(y)$  and  $F_{y|x_i}(y)$  are almost the same, i.e., that the distance between these two statistics is close to zero. This would mean that the amount of output variability reduction because of fixing the value  $x_i$  is negligible, which in turns implies that this parameter has almost no contribution to the output and could well be screened out. Conversely, if the distance of the two CDFs is large, this would mean that almost all the variability of the output can be explained by this parameter. The distance between the UCDF and the CCDF is measured through the Kolmogorov-Smirnov (KS) statistic. Formula 20 defines the KS statistic for a given  $x_i$  value.

$$KS(x_i) = |F_y(y) - F_{y|x_i}(y)| \quad (20)$$

It is important to bear in mind that the KS distance depends on the value upon which it has been conditioned. If we were to use the KS statistic as it is defined in Equation 20, this would mean that the model would be conditional on an assumed value, which is not desirable. The metric could give different results based on the conditioning value. As a way to uncondition the previous definition or remove the dependency of  $x_i$ , a statistic for the KS (for instance, the median) is used.

$$T_i = \text{stat}_{x_i} |KS(x_i)| \quad (21)$$

This index  $T_i$ , shown in Equation 21, has several characteristics: It is global, so the input variations take place in the entire feasible space; it is quantitative, model independent, unconditional, easy to interpret and implement, stable and moment independent. The last property is the main difference between the distribution-based and the variance-based techniques. Considering the fact that the analytical computation of the index  $T_i$  is impossible in most cases, the following numerical techniques attempt to estimate it.

$$\widehat{KS}(x_i) = |\widehat{F_y}(y) - \widehat{F_{y|x_i}}(y)| \quad (22)$$

Equation 22, describes the formulation, where  $\widehat{F_y}(y)$  and  $\widehat{F_{y|x_i}}(y)$  are the empirical UCDF and CCDF approximated by a finite number of samples. Whereas the UCDF is approximated using  $N_u$  output evaluations by sampling the entire output feasibility space, the CCDF is approximated using  $N_c$  output evaluations by sampling all but  $x_i$  inputs. Consequently, the conditional KS can be transformed to an unconditional KS by means of a statistic, as displayed in Equation 23. However, it is important to notice that the choice of conditioning points will have an effect on the result. Both  $T_i$  and  $S_{T_i}$  metrics range from 0 to 1.

$$\widehat{T}_i = \text{stat}_{x_i=x_i^{(1)}, \dots, x_i^{(n)}} |\widehat{KS}(x_i)| \quad (23)$$

The implementation of PAWN has been made available in [22]. This version of PAWN is now considered as the tailored sampling approach method and further information can be found in [7, 23]. More recently in 2018, as mentioned in the introduction, a new implementation of PAWN, called the distribution-based method, addressed the limitations of the old version; this can be found in [13]. The distribution-based method splits the range of variation of each input factor  $x_i$  into  $n$  equally spaced intervals  $I_k$

and define the conditional samples  $YC_{ik}$  accordingly. The unconditional sample  $YU$  can coincide with the entire sample  $Y$  or with a subsample of it. This is represented in Equation 24.

$$\hat{S}_i = \text{stat}_{k=1,\dots,n} KS(I_k) \text{ where } KS(I_k) = |\widehat{F}_y(y) - \widehat{F}_{y|x_i}(y)| \in I_k \quad (24)$$

The main difference between the old and new version of PAWN is shown in Figure 1, sourced from [13]. "Example of using a tailored sampling strategy (left) and generic sampling (right) to approximate the PAWN index of input  $x_1$  in a case of  $M=3$  input factors. Left (tailored): (a) Input samples used to derive the unconditional output sample  $YU$ . These are generated by randomly sampling the entire space of input variability. (b) Input samples used to derive three conditional samples  $YC_{11}$ ,  $YC_{12}$  and  $YC_{13}$ . These are generated by fixing  $x_1$  at selected conditioning values (for the sake of clarity, only  $n=3$  conditioning values are shown here). (c) Scatter plot of the unconditional (red) and conditional (grey) output samples  $YU$ ,  $YC_{11}$ ,  $YC_{12}$  and  $YC_{13}$  against  $x_1$ . Right (generic): similar to the left hand side but this time the input samples in (d) and (e) are the same. A random subset (highlighted in red) is used to derive  $YU$ , and the three subsets obtained by splitting the variability range of  $x_1$  into 3 intervals (grey) are used to derive  $YC_{11}$ ,  $YC_{12}$  and  $YC_{13}$ . After sampling, the approximation of the PAWN sensitivity index follows the same steps: (g) unconditional output distribution (red) and the three conditional distributions (grey) when  $x_1$  is fixed to a given value (interval). (h) KS statistic (maximum absolute difference) between the unconditional distribution and each of the three conditional ones, plotted against the conditioning value (centre of the interval)".

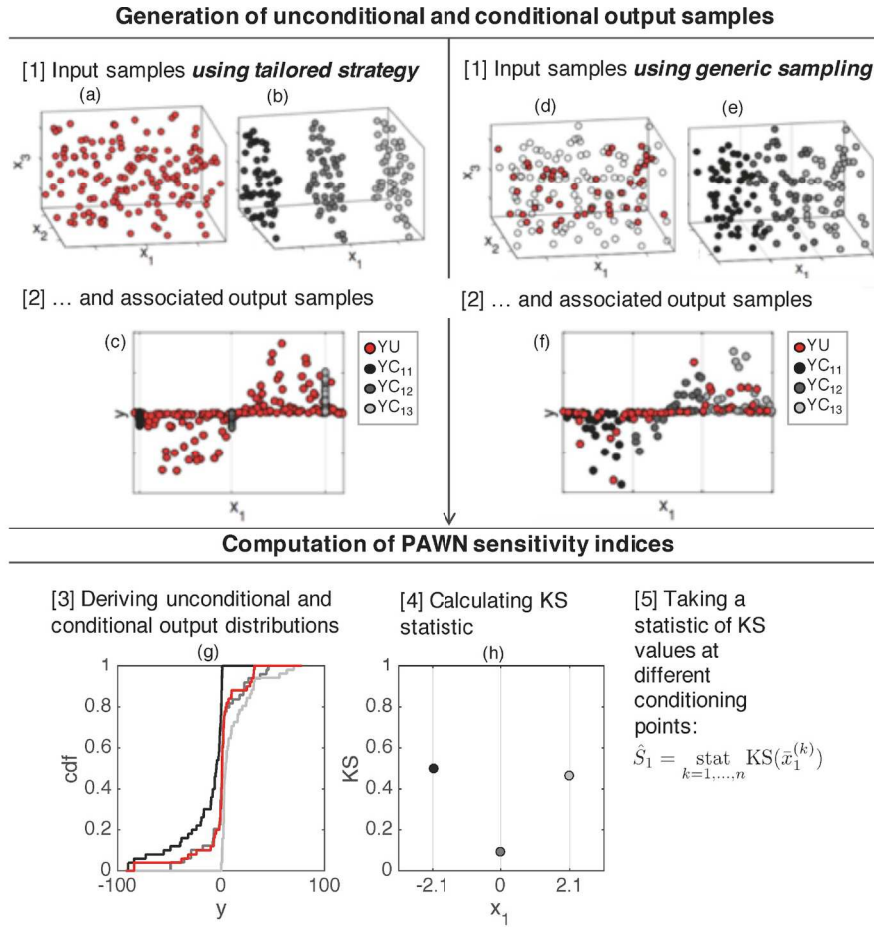


Figure 1: Comparison between the tailored and generic approach for the distribution-based method

## 4 Test Functions

A set of well-studied test functions is investigated to benchmark the distribution-based against the reference VBSA. The following functions are briefly described below for the sake of completeness.

**Function 1:** The Ishigami function is one of the most common benchmark test functions because it exhibits strong non-linearity and non-monotonicity [24], as displayed in Equation 25. It has already been used as a benchmark by the distribution-based method in [13]. Parameters  $a = 7$  and  $b = 0.1$  are assumed and  $X_i \sim U(-\pi, \pi)$ ; its analytical variance is displayed in Table 2.

$$Y = \sin(X_1) + a\sin^2(X_2) + bX_3^4\sin(X_1) \quad (25)$$

$X_i$	ST[%]
1	55.76
2	44.24
3	24.37

Table 2: Analytical variance for Ishigami-Homma test function

**Function 2:** The K function was introduced by Bratley et al. [25] and used for GSA in [18]. The K function is displayed in Equation 26.

$$K = \sum_{i=1}^k (-1)^i \prod_{j=1}^i X_j \quad (26)$$

$X_i$  is uniformly distributed in the interval  $[0,1]$ . In this test function there are few dominant variables:  $X_1$  and  $X_2$  account for most of the uncertainty band. Moreover, the degree of interaction increases with higher index variables due to the construction of the function. The analytical variance is displayed in Table 3.

**Function 3:** The non-additive B function was proposed by Saltelli et al. in [2] and displayed in Equation 27.

$$B = \sum_{i=1}^m X_i \cdot X_{m+i} \quad (27)$$

Where  $m = k/2$  ( $k$  being even),  $X_i \sim N(\overline{X}_i, \sigma_{X_i})$ ,  $i = 1, 2, \dots, k$  and  $N(\overline{X}_i, \sigma_{X_i})$  concerns the mean and standard deviation of a normal distribution. The choice of the different normal distribution parameters condition the number of important factors. Contrary to the  $G^*$  and  $K$  functions, non-relevant parameters have a non-nihil effect. The same parameters as [19] for the B function are kept and shown in Table 3.

**Function 4 & 5:** The  $G^*$  function is a modified version of the G-Sobol function and it was introduced in [18]. This function is shown in Equation 28 and 29.

$$G^*(X_1, \dots, X_k; a_1, \dots, a_k, \delta_1, \dots, \delta_k, \alpha_1, \dots, \alpha_k) = \prod_{i=1}^k g_i^* \quad (28)$$

where  $g_i^*$  is defined as:

$$g_i^* = \frac{(1 + \alpha_i) \cdot |2(X_i + \delta_i - I[X_i + \delta_i] - 1|^{\alpha_i} + a_i}{1 + a_i} \quad (29)$$

Where  $X_i$  are the input factors, uniformly distributed between  $[0, 1]$ ,  $a_i > 0$  are the traditional G functional parameters,  $\delta_i \in [0, 1]$  and  $\alpha_i > 0$  are the shift and curvature parameters, respectively.  $\delta_i$ s are randomly chosen since the uncertainties propagate independently of them. The mathematical meaning of  $I[X_i + \delta_i]$  refers to the integer part of  $X_i + \delta_i$ . It is also worth adding that the relative importance of the factors directly depends on the choice of the parameters. For this reason, two functions are considered for benchmarking purposes with 4 and 10 important factors : 4 ( $G_4^*$ ) and 10 ( $G_{10}^*$ ), whose parameters and analytical variance are displayed in Table 3.

$X_i$	$K$	$B$	$G_4^*$				$G_{10}^*$			
	ST[%]	$\bar{X}_i$	$\sigma_{X_i}$	ST[%]	a	$\alpha$	ST[%]	a	$\alpha$	ST[%]
1	75.00	0	0.5	0.39	100	1	0	100	1	0
2	25.00	0	0.5	0.62	0	4	67.44	0	4	75.49
3	8.33	0	1	1.55	100	1	0	100	1	0
4	2.78	0	1	1.55	100	1	0	100	1	0
5	0.93	0	2	12.41	100	1	0	100	1	0
6	0.31	0	2	22.34	100	1	0	100	1	0
7	0.10	0	1	3.49	1	0.5	3.19	1	0.4	2.56
8	0.03	0	0.5	1.40	0	3	59.28	10	3	1.24
9	0.01	0	1.5	20.25	100	1	0	0	0.8	23.30
10	0	0	2	36.00	100	1	0	0	0.7	20.00
11	0	1	2	0.31	0	2	46.83	9	2	0.94
12	0	2	2	0.31	100	1	0	0	1.3	37.68
13	0	2	1	0.31	100	1	0	100	1	0
14	0	2	1	0.31	100	1	0	100	1	0
15	0	3	1	1.24	1	0.5	3.19	4	0.3	0.26
16	0	3	3	11.17	100	1	0	100	1	0
17	0	1.5	3	2.79	100	1	0	100	1	0
18	0	3	3	0.70	0	1.5	37.94	7	1.5	1.03
19	0	2	5	17.46	100	1	0	100	1	0
20	0	2	5	31.03	1	0.5	3.19	2	0.6	2.11

Table 3: Parameters and analytical variance for  $K$ ,  $B$ ,  $G_4^*$  and  $G_{10}^*$  test functions

**Function 6:** A highly-skewed test function defined in Equation 30 was proposed in [6].

$$y = \frac{x_1}{x_2} \quad (30)$$

Where  $x_1 \sim \chi^2(d_1)$  and  $x_2 \sim \chi^2(d_2)$  follow Chi-square distributions with  $d_1$  equal to 10 and  $d_2$  13.978. The quotient of two Chi-square distributions is F-distributed. Hence analytical values are shown in Table 4 and its formulation is presented in the Appendix for the sake of completeness. If  $d_1$  was 10 and  $d_2$  14, the ST would be 54.5454% for both inputs. However, it has been purposely chosen to set  $d_2$  smaller than 14 so that the theoretical variance of input factor 2 is greater than input factor 1.

$X_i$	ST[%]
1	54.50
2	54.60

Table 4: Analytical variance for highly-skewed test function

## 5 Results and Discussion

### Ishigami-Homma function:

In order to allow for a fair comparison between the VBSA and the distribution-based, the same number of model evaluations is considered. The benchmark is carried out by taking the distribution-based with  $N = 5000$  and  $n = 20$  against VBSA with  $N = 1250$  samples. Both result into approximately 5000 model evaluations. Results are displayed in Figure 2. Total sensitivity indices  $ST_i$  (small circles in red) are estimated via Monte Carlo method (by means of the Sobol low-discrepancy sequence) for input factors  $X_i$   $i = 1, \dots, 3$ . 95 % confidence intervals (vertical dashed lines in red) are estimated by bootstrapping 1000 replicas. Analytical variances (crosses in magenta) are given for all input factors. Total Kolmogorov Smirnov (KS) statistics  $T_i$  (small circles in blue) are estimated via random Monte Carlo sampling. 95 % confidence intervals (vertical dashed lines in blue) are estimated by bootstrapping 1000 replicas. The level of noise for the distribution-based method (horizontal dashed lines in blue) is calculated by the introduction of a dummy variable. This level of noise is bootstrapped 1000 times and results into the upper and lower horizontal dashed lines in blue. This means that, if the  $T_i$  was comprised between the upper and lower bound, we wouldn't be able to say if this is due to the importance of the input or the level of noise of the method.

Figure 2 also shows that the analytical variance is inside the confidence level for the variance-based method. If we were to rank the importance of the inputs based on the two measures, we would obtain different results - the distribution-based method captures the non-linearity of the second input factor  $X_2$  and places more weight on its uncertainty than the variance-based method. Also, the distribution-based method is not able to capture the importance of  $X_2$  as it falls below the upper level of noise. A convergence analysis in VBSA is conducted by increasing the sample size from 125 to 2500 by steps of 125. In addition to this, 95 % confidence intervals are estimated by bootstrapping 1000 replicas in each case. This is shown in Figure 3(a). The same process is repeated for the distribution-based. Whereas the left axis is used for Sobol with  $ST_i$ , the right one is used for distribution-based with  $T_i$ . The number of conditioning points has been kept to 20, whereas  $N$  is increased from 500 to 10000 by steps of 500, as shown in Figure 3(b). As expected, when we increase the number of samples, the range of the confidence intervals is reduced.  $ST_i$  and  $T_i$  remain stable for the Ishigami-Homma function across the different simulations.

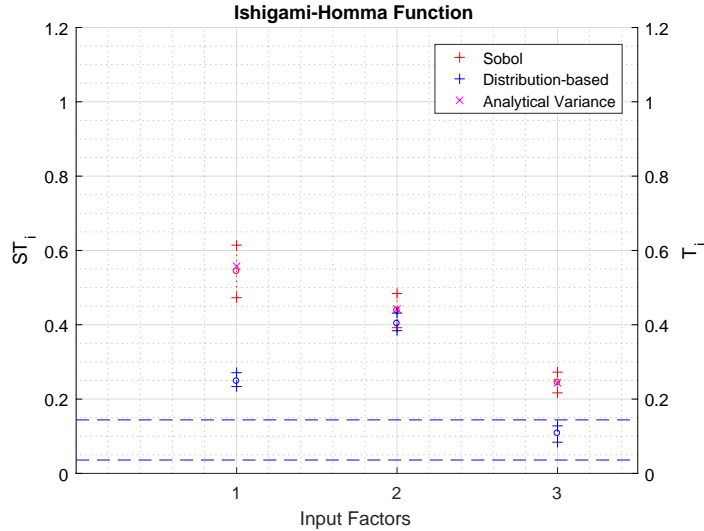


Figure 2: Benchmarking the distribution-based with  $N = 5000$   $n = 20$  and  $k = 3$  against VBSA with  $N = 1250$  samples. Both result into 5000 model evaluations.

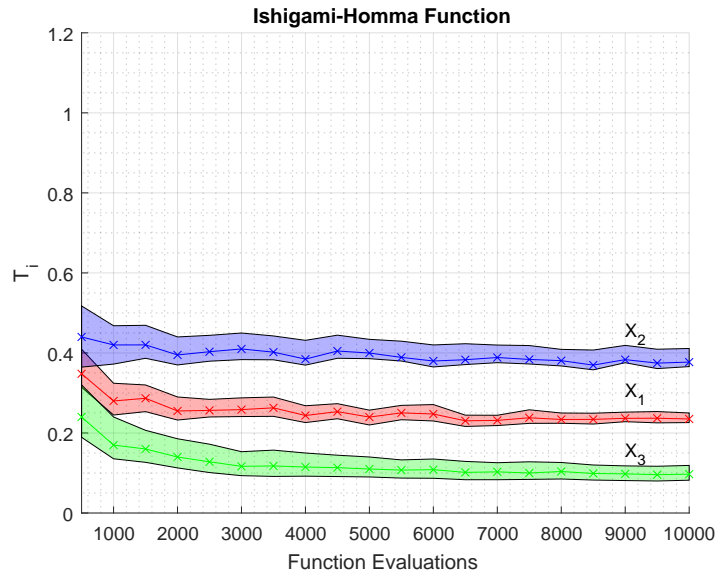
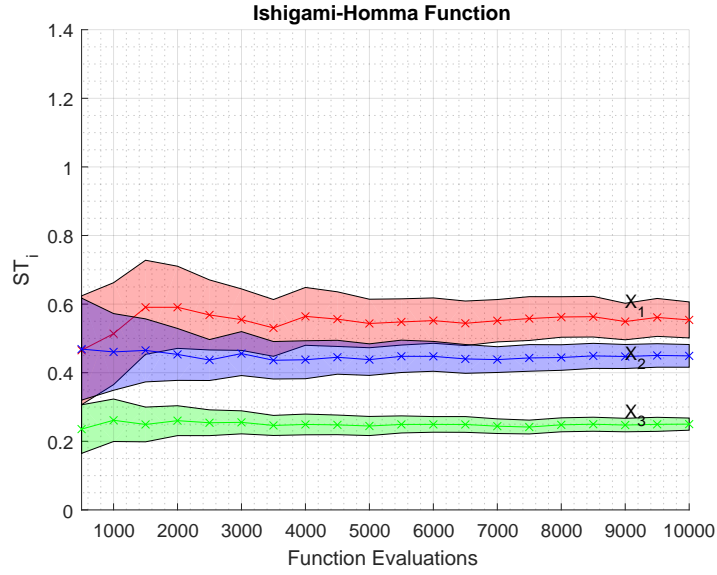


Figure 3: Coverage analysis for Ishigami-Homma function. Comparison of distribution-based  $T_i$  and Sobol  $S_i$  indices for input factors  $X_1$ ,  $X_2$  and  $X_3$ . (a): VBSA (b): distribution-based

**K, B  $G_4^*$  and  $G_{10}^*$  function:**

The same number of model evaluations is considered for the following 4 functions in order to allow for a fair comparison between the VBSA and the distribution-based . The benchmark is carried out by taking the distribution-based with  $N = 25200$  and  $n = 20$  against VBSA with  $N = 1200$  samples. Both result into approximately 25200 model evaluations. Results are displayed in Figure 4. Total sensitivity indices  $ST_i$  (small circles in red) are estimated via Monte Carlo (by means of the Sobol low-discrepancy sequence) for input factors  $X_i$   $i = 1, \dots, 20$ . 95 % confidence intervals (vertical dashed lines in red) are estimated by bootstrapping 1000 replicas. Analytical variances (crosses in magenta) are given for all input factors. Total Kolmogorov Smirnov (KS) statistics  $T_i$  (small circles in blue) are estimated via random Monte Carlo sampling. 95 % confidence intervals (vertical dashed lines in blue) are estimated by bootstrapping 1000 replicas. The level of noise for the distribution-based method (horizontal dashed lines) is calculated by the introduction of a dummy variable. This level of noise is bootstrapped 1000 times and results into the upper and lower horizontal dashed lines in blue, as previously done for the Ishigami - Homma test function.

As far as the K function is concerned, only the first 9 inputs contribute to the variance of the output, which is reflected in Table 2. Input  $X_1$  has a greater contribution than  $X_2$  and  $X_2$  has a greater contribution than  $X_3$ , and so on and so forth. However, when the distribution-based method is used, only  $X_{1,2,3}$  can be considered within the validity of the method. The level of noise of the method doesn't allow us to say, for example, that input  $X_4$  has a greater contribution than input  $X_{15}$ . Consequently, the method fails to rank inputs that have different order of magnitude in the contribution of the response. When applied to the B function, the distribution-based method allows to identify  $X_{5,6,9,10}$  but fails to rank three of the most relevant contributors to the variance:  $X_{16,19,20}$ . As for the  $G_4^*$  function, the distribution-based method allows to identify  $X_{2,8,11,18}$  but it does not capture the small contributions represented by  $X_{7,15,20}$ . Finally as far as the  $G_{10}^*$  function is concerned, the distribution-based method allows to identify  $X_{2,9,10,12}$  but it doesn't capture the small contributions represented by  $X_{7,8,11,15,18,20}$ .

Figure 4 also shows that the analytical variance is inside the confidence level in VBSA for all but one input factor -  $X_{11}$  from the B function. It has been checked that increasing the number of model evaluations leads to the analytical variance falling inside the confidence level for all input factors. A convergence analysis in VBSA is conducted by increasing the sample size from 60 to 1200 by steps of 60, leading to a total of 25200 model evaluations in the last case. Confidence intervals are estimated by bootstrapping 1000 replicas in each case. Whereas Figure 5 doesn't display the confidence interval for a better interpretation, Figure 6 does display it for its main three inputs resulting. The same process is repeated for the distribution-based. The number of conditioning points has been kept to 20, whereas  $N$  is increased from 1260 to 25200 by steps of 1260, as shown in Figure 5(b,d).  $ST_i$  remain stable for both the K and B Function across the different simulations.  $T_i$  is also stable and changes only occur in  $X_5$  and  $X_6$  for the B function, as they have similar KS values. This is basically due to the fact that the 20 conditioning points ( $n$ ) play a role in exploring the search space. These conditioning points are evenly spaced within the domain, but change from simulation to simulation. Finally, it is also worth noticing that in Figure 6(d) the main input factors from Sobol cannot be recognised in function B once the confidence levels are plotted.



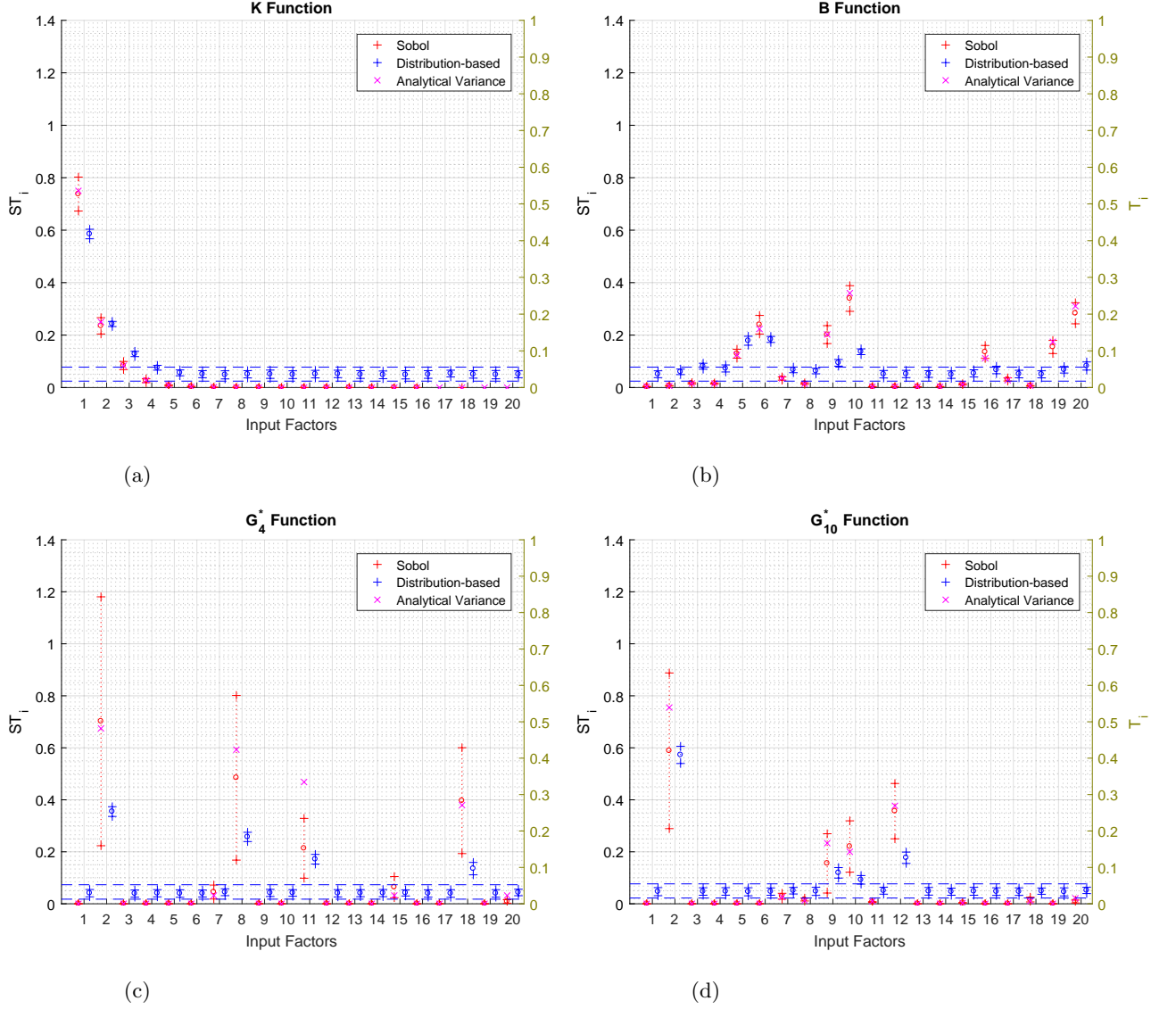


Figure 4: Benchmarking the distribution-based with  $N = 25200$  and  $k = 20$  against VBSA with  $N = 1200$  samples. Both result into 25200 model evaluations. (a): K Function (b): B Function (c):  $G_4^*$  Function (d):  $G_{10}^*$  Function

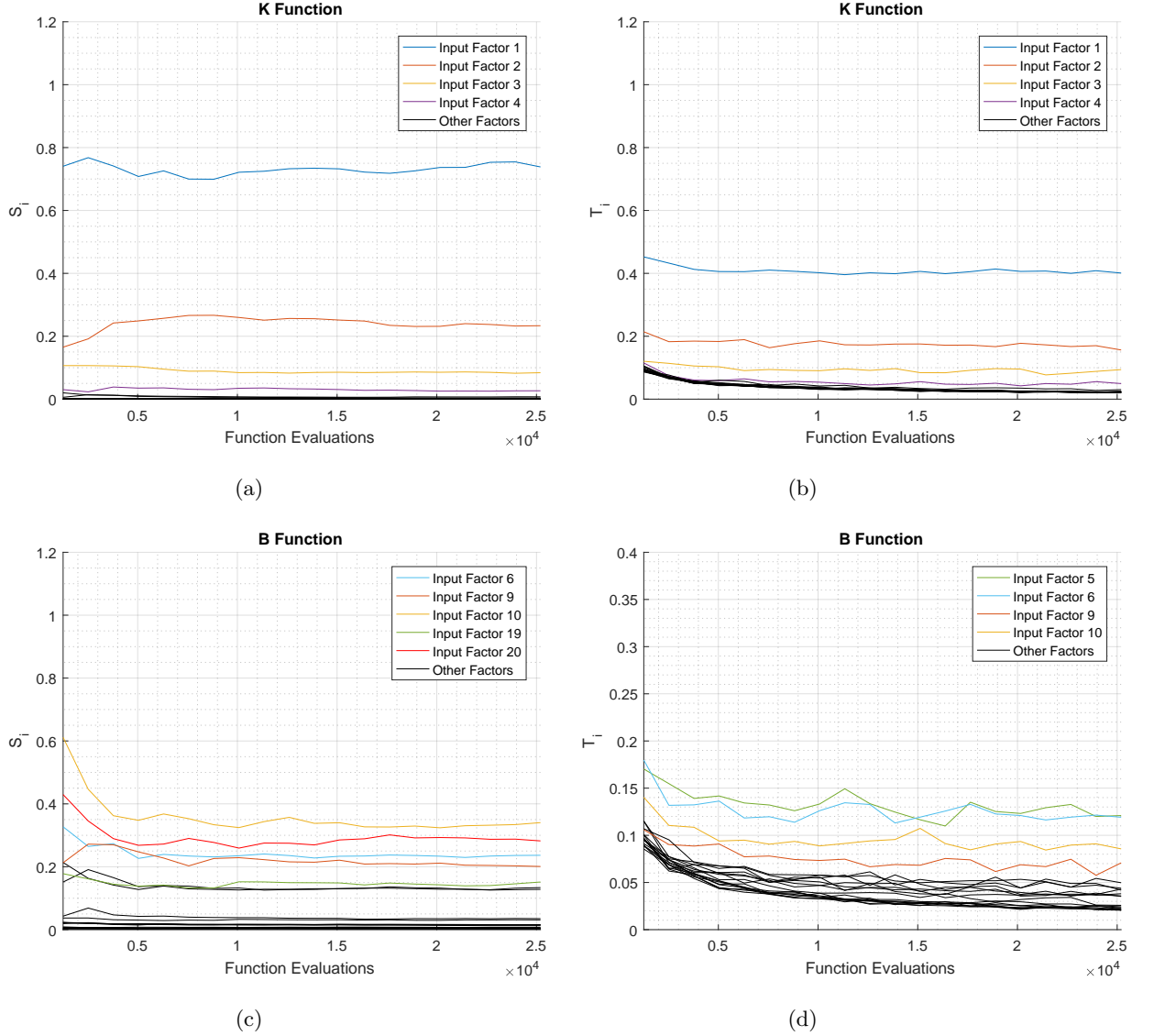


Figure 5: Convergence analysis for K Function (a,b) and B Function (c,d). Comparison of distribution-based  $T_i$  and Sobolj  $S_i$  indices.(a,c): VBSA (b,d): distribution-based

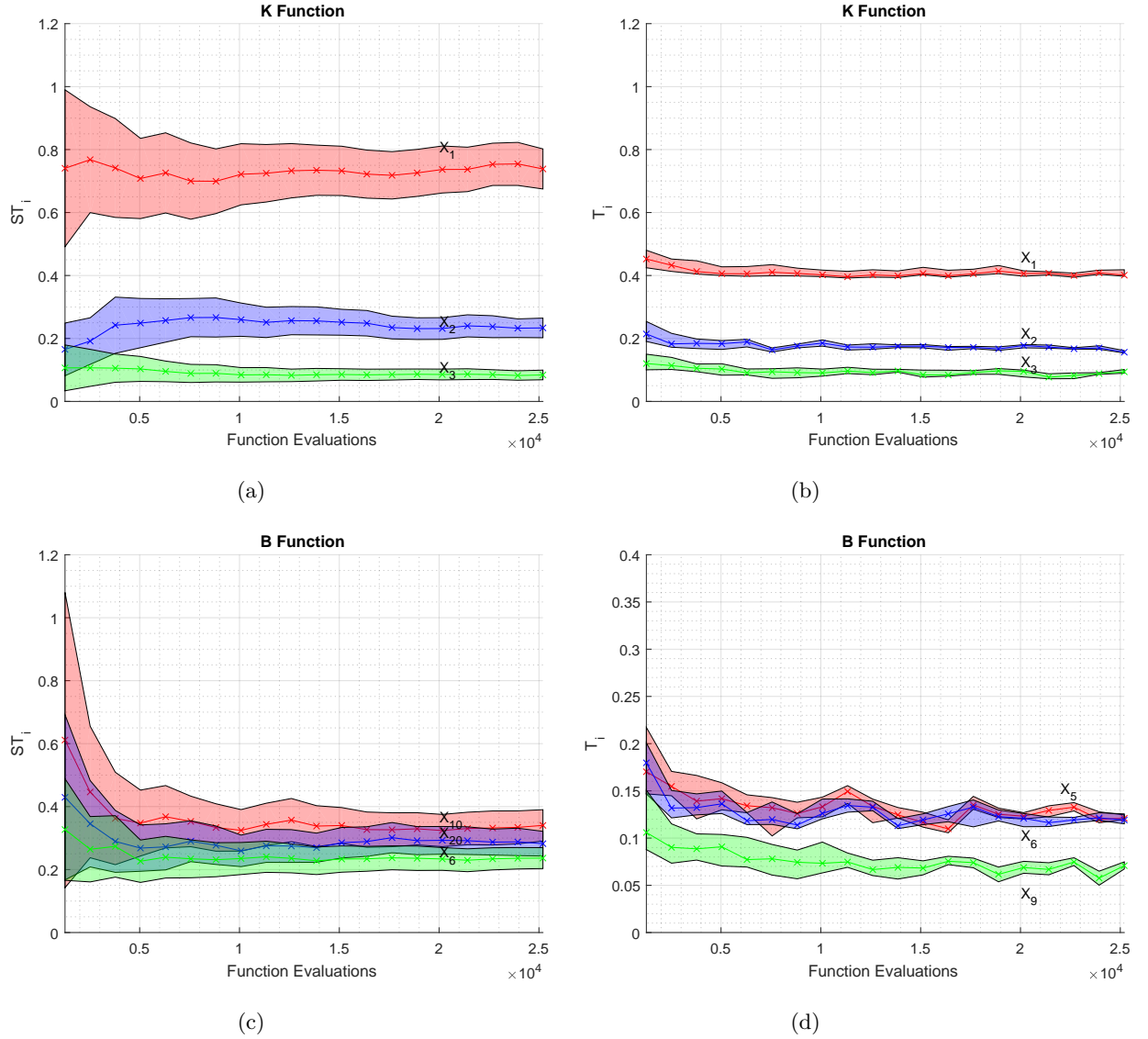


Figure 6: Convergence analysis for K Function (a,b) and B Function (c,d) for its three main inputs. Comparison of distribution-based  $T_i$  and Sobol  $S_i$  indices. (a,c): VBSA (b,d): distribution-based

### Highly skewed function:

The empirical PDF of the highly-skewed function (Equation 30) is displayed on the left hand side of Figure 7, together with the associated scatter plots which confirm the importance of  $X_1$  over  $X_2$ , as studied in [6].

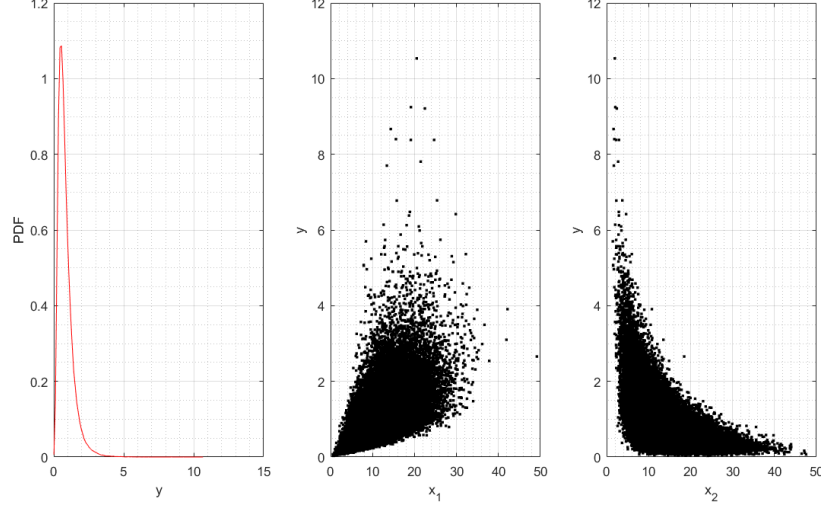


Figure 7: Empirical PDF of Function 6 and associated scatter plots with 100000 samples

Figure 8 shows a convergence analysis for the same highly-skewed function using the VBSA and the distribution-based. 95% confidence intervals are represented with coloured patch. It is seen that whereas the Sobol method shows that  $X_1$  and  $X_2$  input factors are equally important, the distribution-based generally recognises the input factor importance  $X_1$  over  $X_2$ , as it is shown in [7]. A convergence analysis in VBSA is conducted by increasing the sample size from 400 to 8000 by steps of 400, leading to a total of 24000 model evaluations in the last case. Distribution-based convergence analysis is carried out in a similar way with 10 conditioning points.

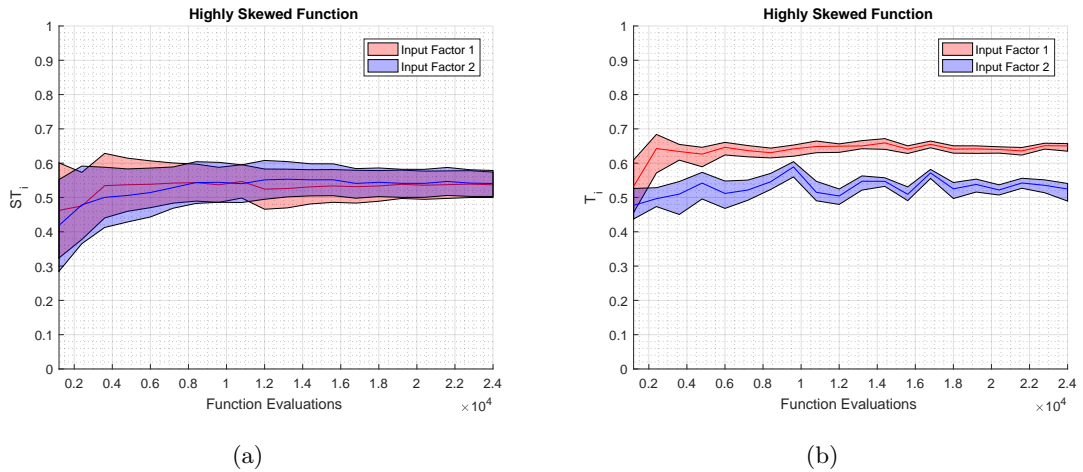


Figure 8: Convergence analysis of PAWN  $T_i$  and Sobol  $S_i$  indices for a highly-skewed function. (a): VBSA (b): distribution-based

### Discussion:

From the results it is clear that the distribution-based method has an inherent high level of noise. A dummy variable  $X_d$  is considered to assess the level of noise for both methods. When assuming a dummy variable for the VBSA method, matrix  $A$  and  $A_B$  differ in column  $B$ . If column  $B$  contains a dummy variable, then, when evaluating the response of the model  $y_A$ , this will be equal to  $y_{A_B}$ , resulting in a nil contribution to the variance, as shown in Equation 31. Therefore there is no inherent level of noise associated with the variance-based method.

$$\mathbf{E}_{\mathbf{X}_{\sim i}}(\mathbf{V}_{X_i}([Y|X_{\sim i}])) = \frac{1}{2N} \sum_{j=1}^N [y(a_1^{(j)}, a_2^{(j)}, \dots, a_k^{(j)}) - y(a_1^{(j)}, a_2^{(j)}, \dots, b_i^{(j)}, \dots, a_k^{(j)})]^2 \quad (31)$$

On the other hand, the distribution-based's difference between the UCDF and CCDF provides a metric as to how important an input is. Even if the two CDFs were the same - under the assumption of a dummy variable - the fact that the variable must be conditioned results into a level of noise. However, since we expect the input samples to be uniformly spread in the given dataset we may also expect the size of the conditional sample to be approximately equal to  $N/n$ . This means that the user is able to increase the resolution of the conditional sample at the expense of a higher computational cost by controlling both  $N$  and  $n$ . This rationale is tested on the Ishigami-Homma function. The level of noise is measured by the mean of the KS statistic, which is in turn based on the maximum distance of several conditioning points; this is displayed in Equation 32.

$$\widehat{T}_{dummy} = \text{mean}_{1,2,\dots,n} \max | \widehat{F}_y(y) - \widehat{F}_{y|x_i}(y) | \quad (32)$$

Figure 9 shows the distribution-based indices for the three input factors of the Ishigami-Homma function. Each subplot report results for one input factor. Indices are approximated using an increasing sample size  $N$  and increasing number of conditioning intervals  $n$ . For each combination of  $(N,n)$ , bootstrapping is used to estimate the 95% confidence interval (vertical line) and mean value (circle) of each distribution-based index. Dashed lines show the KS of the dummy parameter at each combination of  $(N,n)$ . The number of conditioning points bears almost no effect as long as  $n$  is greater than 5; this figure has been reproduced from the work of [13], changing the Ishigami-Homma parameters as defined in the test function.

Furthermore, the computational complexity of the VBSA and distribution-based methods is displayed in Equation 33 and 34, where  $N$  is the number of samples,  $n$  is the number of conditioning points for the distribution-based method and  $k$  is the number of model inputs.

$$F_{eval} = N * (k + 1) \quad (33)$$

$$F_{eval} = N \quad (34)$$

Given that the aim of the paper is to allow for a fair benchmark between the two methods, the total number of model evaluations has been kept the same in all the cases. One of the main advantages of the distribution-based method is that it does not require tailored evaluations of the model; in other words, given an input-output sample is possible to determine the  $T_i$  coefficients.

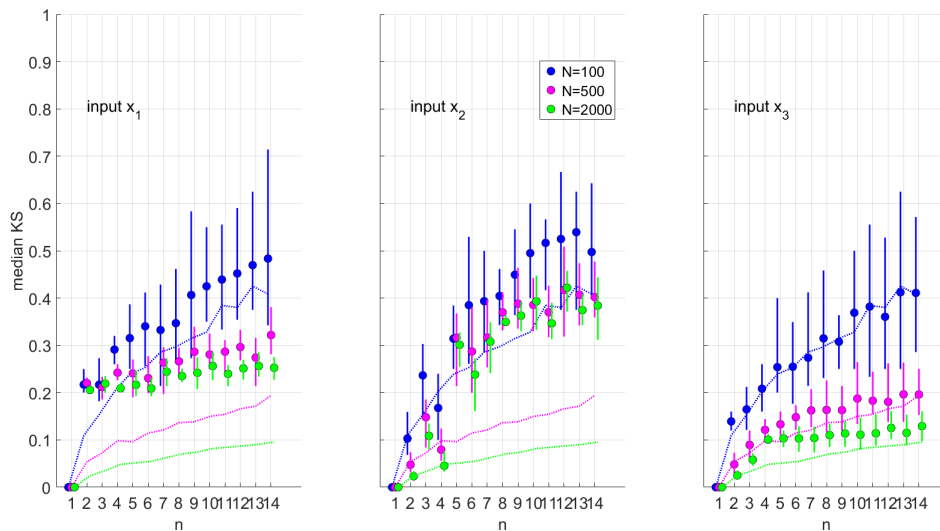


Figure 9: Level of noise as a function of conditioning points and number of samples

## 6 Conclusions

Global sensitivity analysis such as the variance-based and distribution-based methods are widely adopted by the research community in order to identify key input drivers. However, in order for the results to be reproducible all parameters used in either method need to be provided. In addition, bootstrapping should be used to assess the confidence intervals and, where the computational complexity of the problem allows for it, a convergence analysis should be conducted. Given a set of model evaluations, the distribution-based method can be applied at no extra cost, adding value to the global sensitivity analysis and complementing the variance-based method. This paper benchmarks establish a framework on how methods should be compared against each other. It also shows that while the distribution-based method can be used as a complementary approach to the variance-based, as it has the potential to characterise those probability functions that are highly-skewed or multi-modal, it fails to rank different inputs when these have different order of magnitude in their contribution of the response. This has been documented by using well-established test functions, whose analytical variances are known.

## 7 Future work

Future work will focus on adding the CDF-based measure following the ideas of Gamboa, Klein and Lagnoux (2018): “Sensitivity analysis based on Cramér–von Mises distance”, which augments the Sobol’ method with a CDF-based indicator [14]. Gamboa et al. investigated in 2018 the generalisation of the so-called Sobol indices to higher moments, where its index appears to be more general than Sobol as it takes into consideration the whole distribution and not the second moment.

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## 9 Appendix

Analytical variances for the Ishigami-Homma function can be found in [26], whereas analytical variances for the K, B and G\* functions are given in the work of [18]. This appendix includes the analytical variances for the highly-skewed test function, where  $x_1 \sim \chi^2(d_1)$  and  $x_2 \sim \chi^2(d_2)$  follow chi-square distributions with  $d_1$  and  $d_2$  degrees of freedom.

$$y = \frac{x_1}{x_2}$$

Then, if we assume that  $U_1$  is a chi-square distribution with  $d_1$  degrees of freedom,  $U_2$  is a chi-square distribution with  $d_2$  degrees of freedom, and that  $U_1$  and  $U_2$  are independent. The distribution of

$$Y = \frac{U_1/d_1}{U_2/d_2}$$

is F-distributed with  $d_1$  degrees of freedom in the numerator and  $d_2$  degrees of freedom in the denominator. The total variance can be calculated as:

$$V(Y) = \frac{2d_2^2 \cdot (d_1 + d_2 - 2)}{d_1 \cdot (d_2 - 2)^2(d_2 - 4)} \text{ if } d_2 > 4$$

Using the independence property between  $U_1$  and  $U_2$ , the moment generating function of the chi-square distribution as well as some of the properties of the gamma function below:

$$E[U_2^{-1}] = \frac{1}{d_2 - 2}$$

$$E[X^k] = 2^k \frac{\Gamma(n/2 + k)}{\Gamma(n/2)}$$

$$\Gamma(n) = (n - 1)\Gamma(n - 1)$$

Total sensitivity indices  $S_{T_i}$  can be calculated as the sum of first order indices  $S_i$  together with the interactions between the two variables:

$$S_{T1} = S_1 + S_{12} = \frac{d_2 - 4}{d_1 + d_2 - 2} + \frac{2}{d_1 + d_2 - 2} = \frac{d_2 - 2}{d_1 + d_2 - 2}$$

$$S_{T2} = S_2 + S_{12} = \frac{d_1}{d_1 + d_2 - 2} + \frac{2}{d_1 + d_2 - 2} = \frac{d_1 + 2}{d_1 + d_2 - 2}$$



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